LA-UR- 02-7027

Approved for public release;
distribution is unlimited.

Title:

Ultrafast X-ray Diffraction for Measurements of Structural Dynamics in Shocked Metals

Author(s):

Jonathan B. Workman P-24
Paul Keiter P-24
George A. Kyrala P-24
Jeff P. Roberts MST-10
Antoinette J. Taylor MST-10
David J. Funk DX-2

Submitted to:

APS 44th Anunual Meeting Division of Plasma Physics
November 11-15, 2002
Orlando, FL

Los Alamos
NATIONAL LABORATORY

Abstract Submitted
For the DPP02 Meeting of
The American Physical Society
November 11-15, 2002
Orlando, FL

Sorting Category: (Experimental)

Ultrafast X-ray Diffraction for Measurements of Structural Dynamics in Shocked Metals[1] Jonathan Workman, Paul Keiter, George A. Kyrala, Jeff Roberts, Toni Taylor and David J. Funk *Los Alamos National Laboratory* An experiment on structural dynamics at the ultrafast time scale in shocked metal samples is presented. The technique development of an ultrafast x-ray diffractometer to generate "molecular movies" is described. Preliminary results of static x-ray measurements of thin unshocked Ga samples are presented. Initial experiments use 200-300 mJ of a 100fs Ti:Sapphire laser to excite K-alpha x-ray emission in an aluminum wire. The x-ray emission is relayed using a spherical crystal to the sample target. Plans for experiments using Cu K-alpha emission will also be described.

Prefer Poster Session

Jonathan Workman
workman@lanl.gov
Los Alamos National Laboratory

[1] Work performed under the auspices of the Dept. of Energy under contract # W-7405-ENG-36.

Ultrafast X-ray Diffraction for Measurements of Structural Dynamics in Shocked Metals

Jonathan Workman (P-24),

Paul Keiter, George A. Kyrala, Jeff Roberts, Toni Taylor and David J. Funk

Los Alamos National Laboratory

Presented at APS-DPP 2002

Orlando, FL

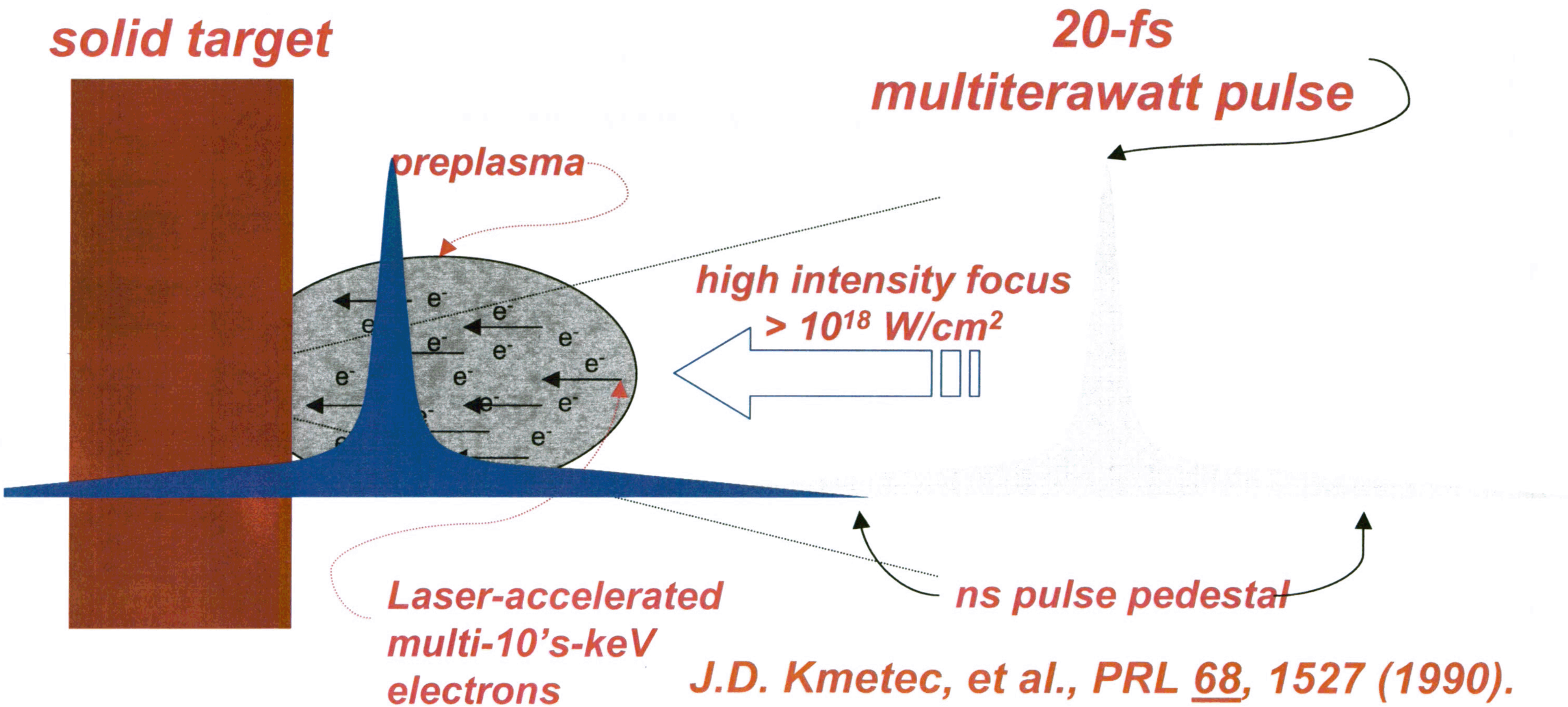
Practical Results from Ultrafast X-ray Diffraction

- Apply X-ray diffraction to shock physics
  - Determine time scales and dynamics of both solid-solid and solid-melt phase changes
  - Develop MD/X-ray capability to both guide experiment (location of X-ray transients) and enhance mechanistic understanding, leading to predictive capabilities
- Apply X-ray diffraction to next generation electronic materials
  - Coherent phonon generation and propagation
  - Study electron-phonon coupling dynamics

Why Ultrafast X-ray Diffraction?

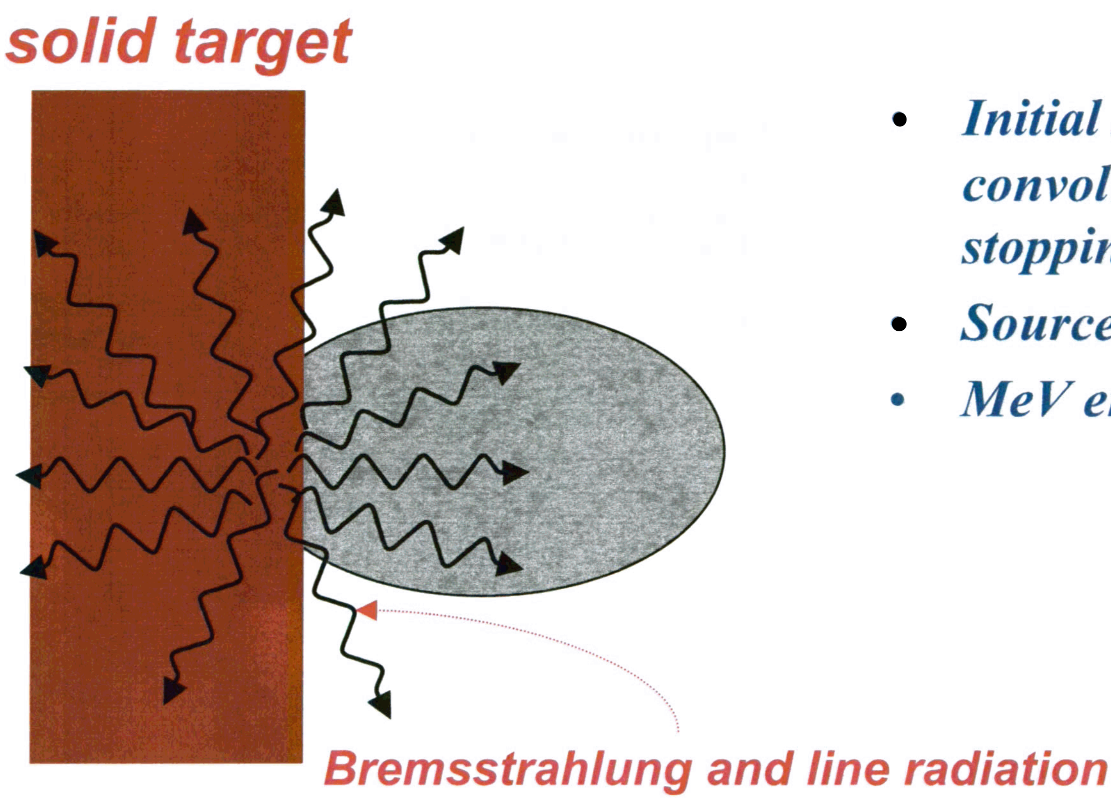
- Ultrafast pump-probe diffraction
  - The synchronicity of laser drive/excitation coupled to thin crystals offers the only opportunity for diffraction on atomic time scales
- Example: Shock waves on the atomic scale
  - Typical velocities are: 7 mm/μs; 7 μm/ns; 7 nm/ps; 0.7 Å/10 fs: *a bond every 50 fs*
- Shock wave characterization
  - What is the risetime? Are their elastic precursors? Do phase changes occur and on what time scales? Ultrafast X-ray diffraction can help answer these and related questions
- Electron-phonon dynamics (ps time scale)
  - Pump electrons, observe lattice motion, observe electron-phonon coupling dynamics
- Perturb 3-D CDW states (ps time scale)
  - Create electron-hole pair, observe lattice relaxation
- Quasi-particle relaxation dynamics (ps time scale)
  - Break Cooper pairs, observe phonon dynamics

Non-Thermal Plasmas Efficiently Generate Short Pulse K_α X-rays



J.D. Kmetec, et al., PRL 68, 1527 (1990).

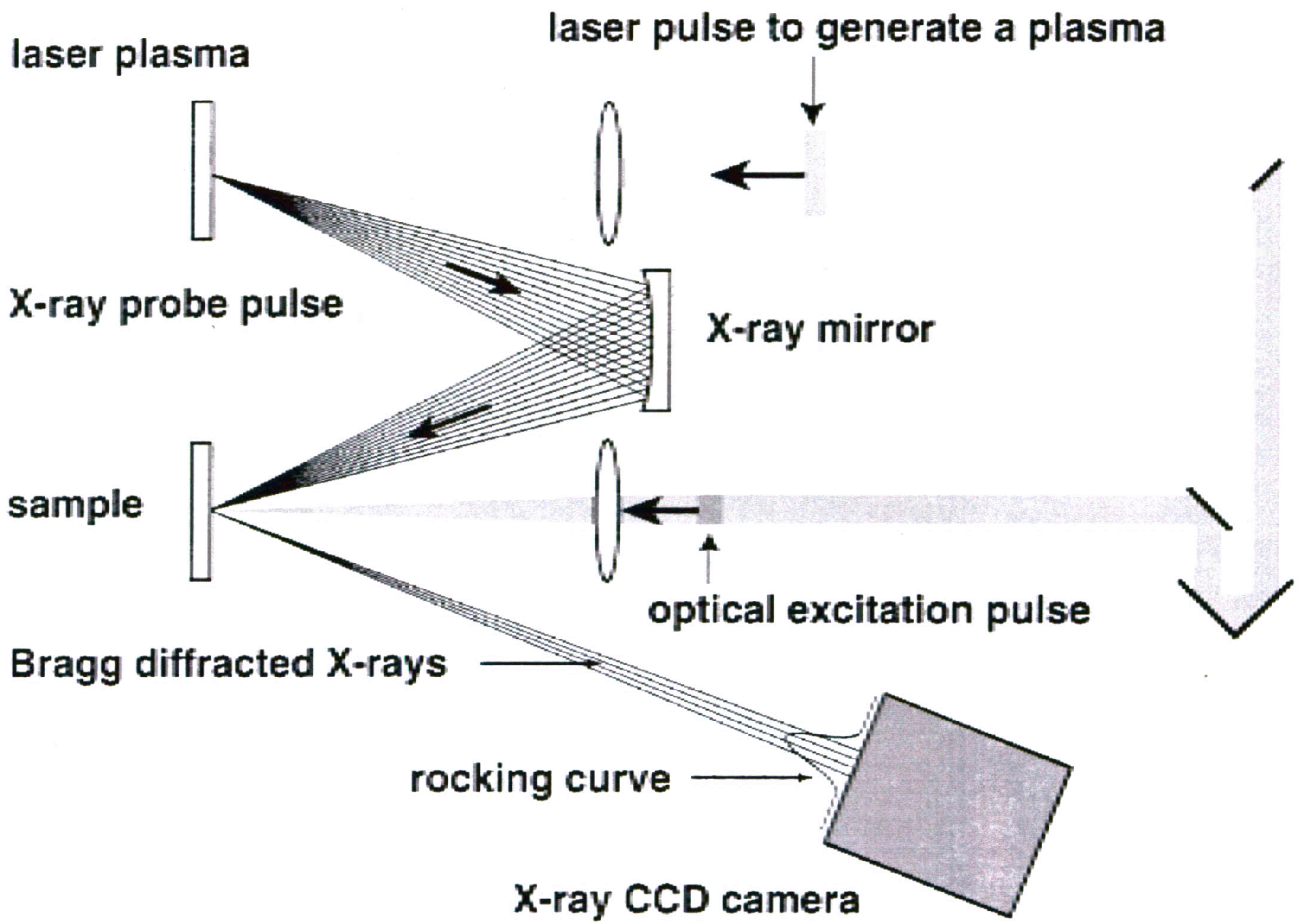
Laser-driven Electrons for Fast X-rays



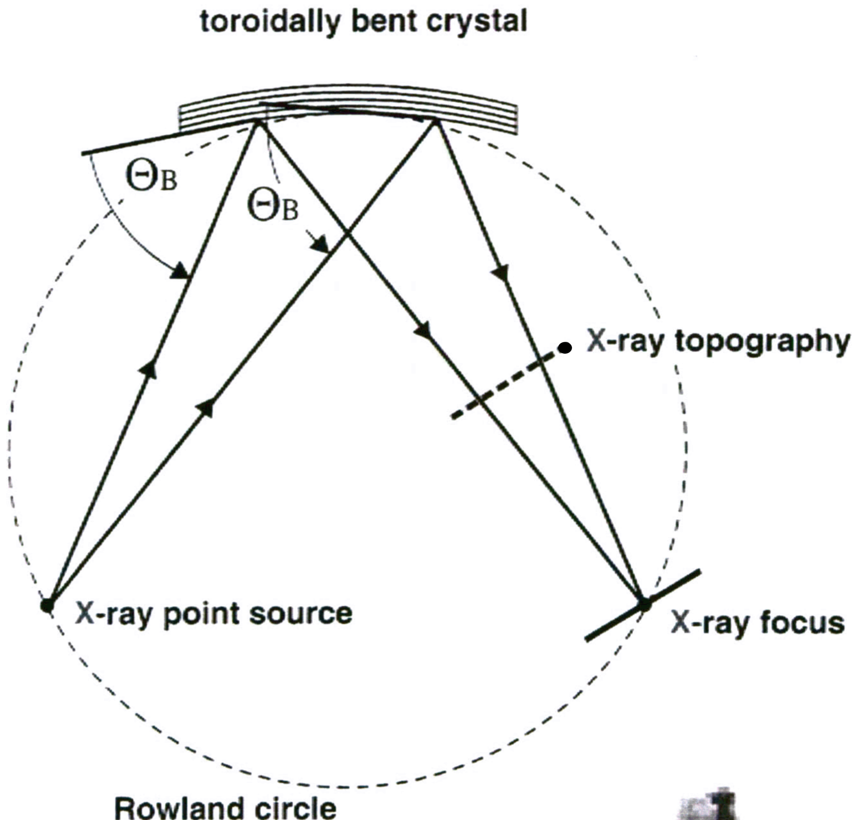
- *Initial x-ray duration: convolution of $\Delta t_{electron}$ and stopping time or emission volume*
- *Source size ~ laser spot size*
- *MeV energies can be produced*

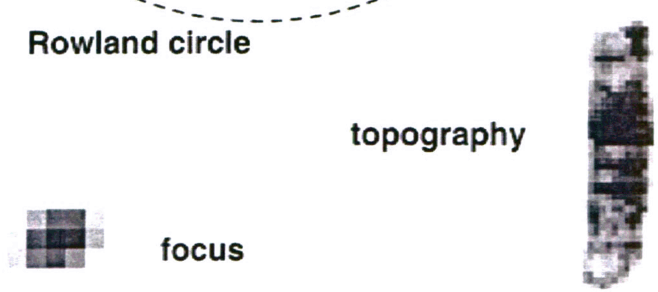
J.D. Kmetec, et al., PRL 68, 1527 (1990).

Ultrafast X-ray Diffractometer Uses a Relay Optic for X-ray Focussing



Use of Toroidal X-ray Optics Optimizes Focusing

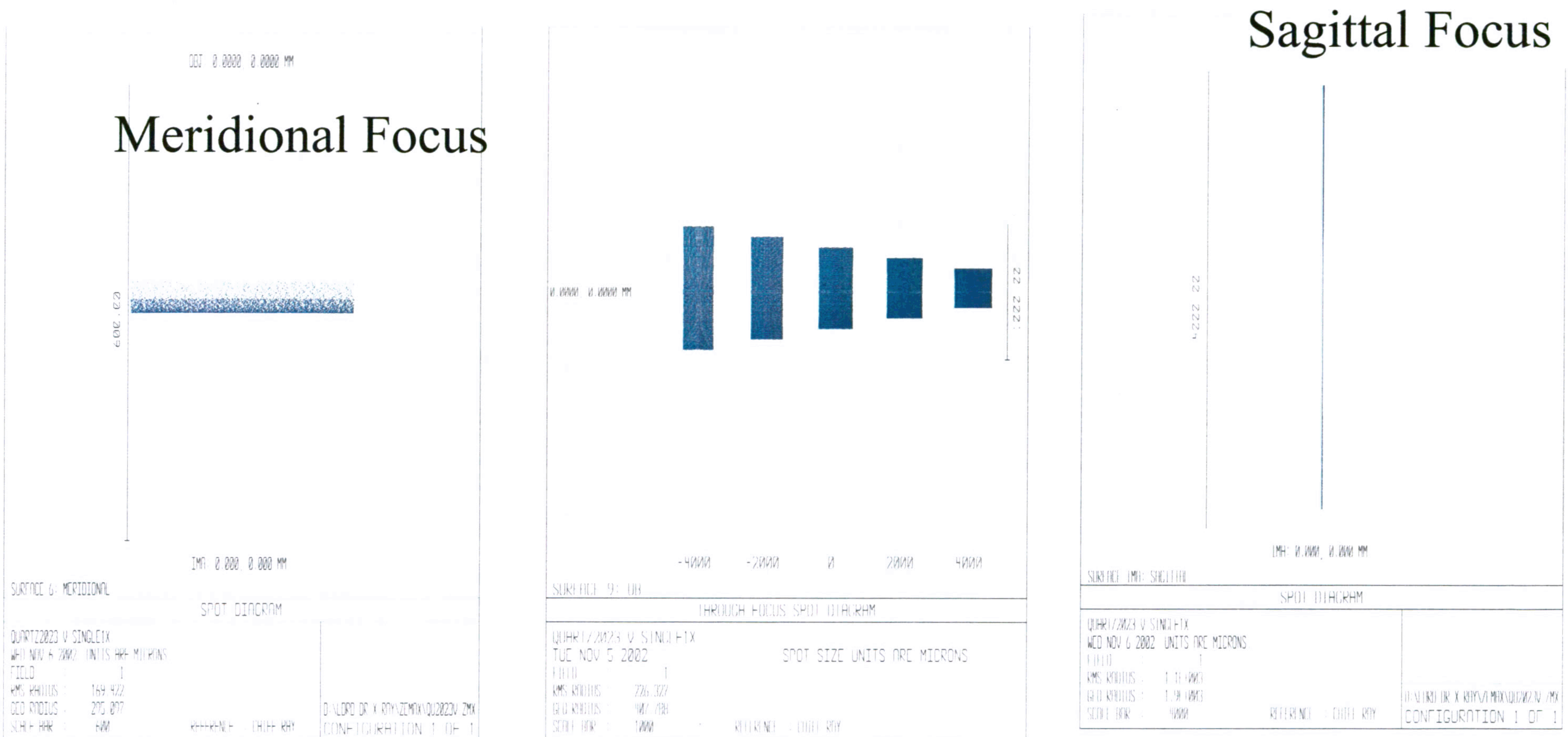




- Two radii of curvature allows for non-normal incident x-rays to focus to nearly a point.

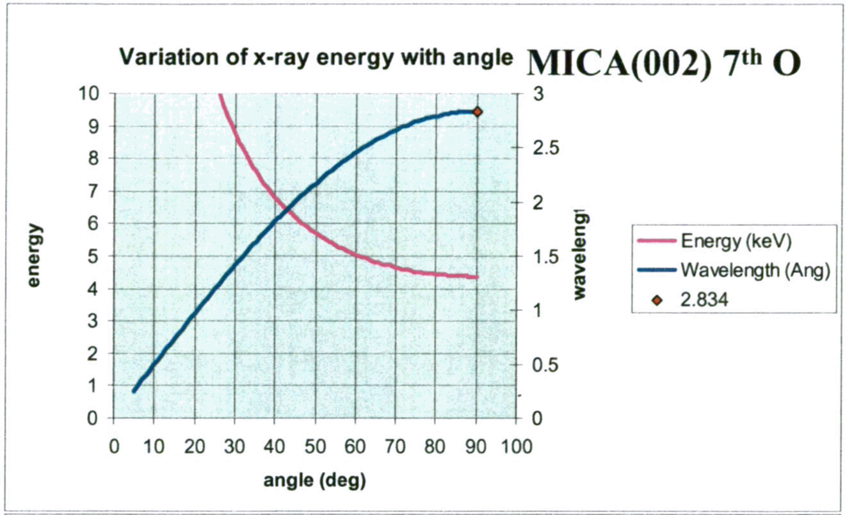
- 1 to 1 magnification allows for greatly increased collection as well as localized probing.

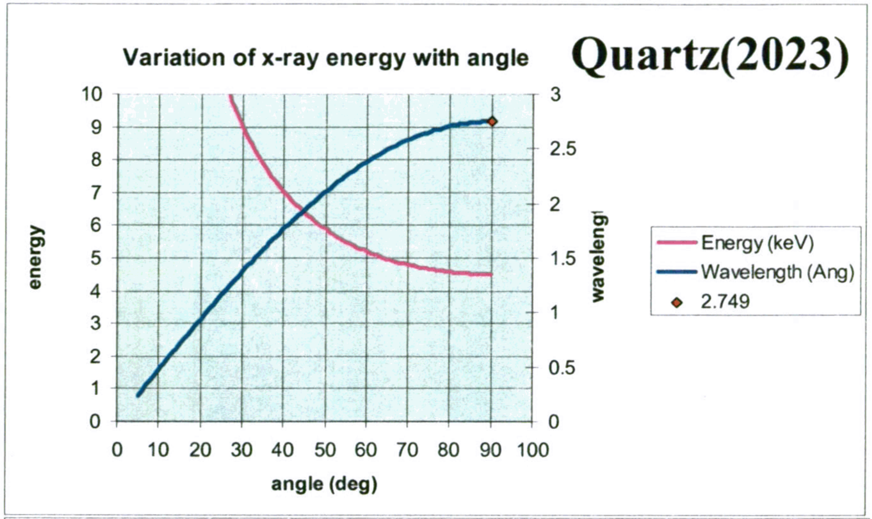
Spherical Crystals Can Also Provide Relay Imaging for Ultrashort X-ray Sources

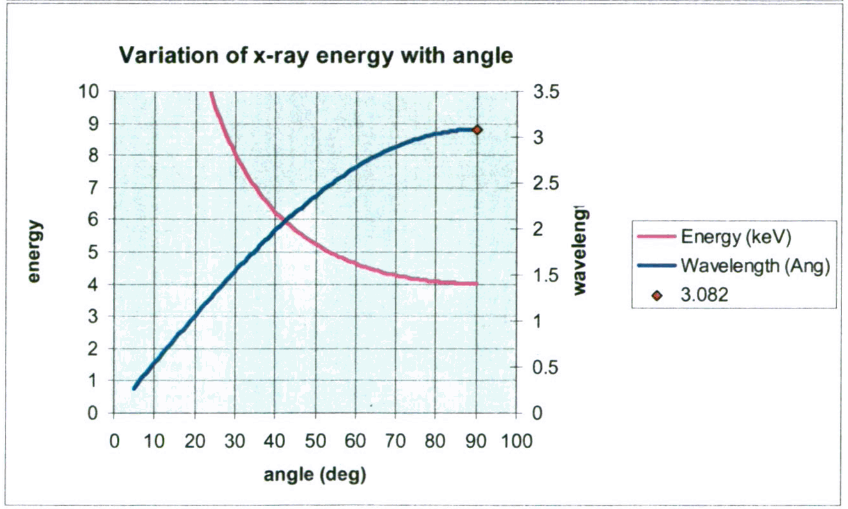


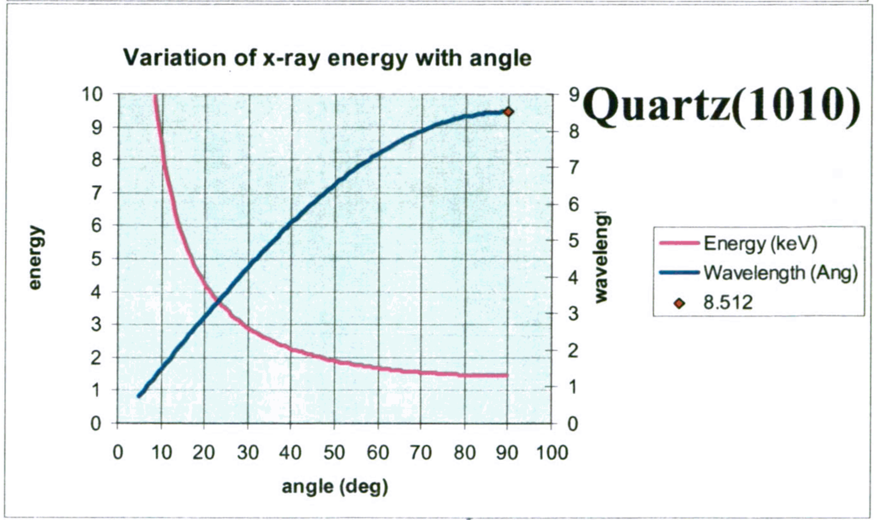
- **Want to Maximize Bragg angle to Minimize astigmatism from Spherical Crystal**

Several Spherical Crystals are Being Considered

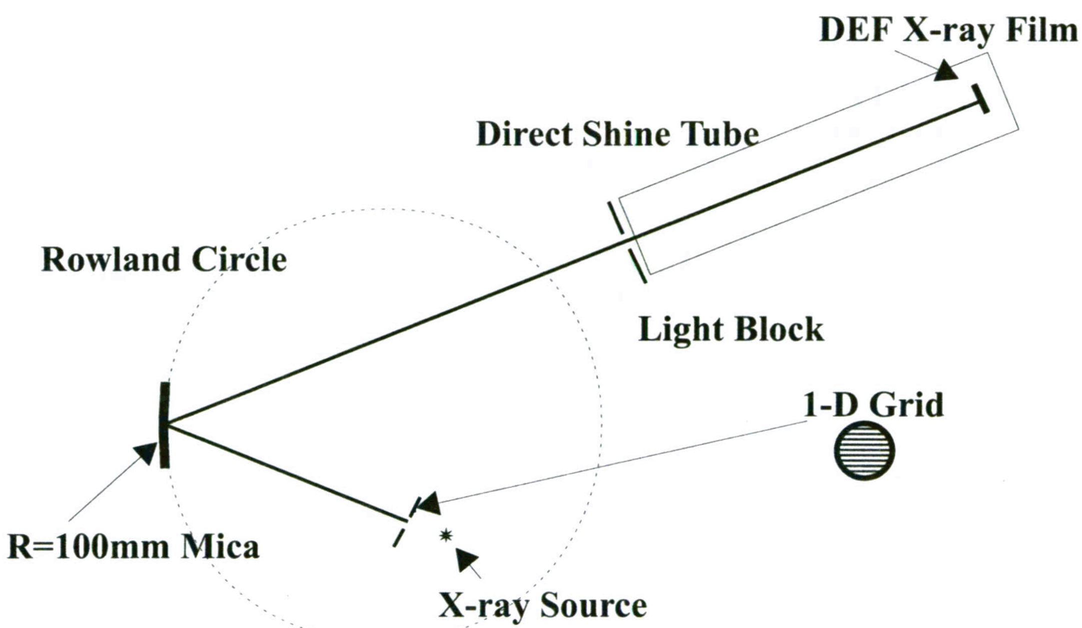


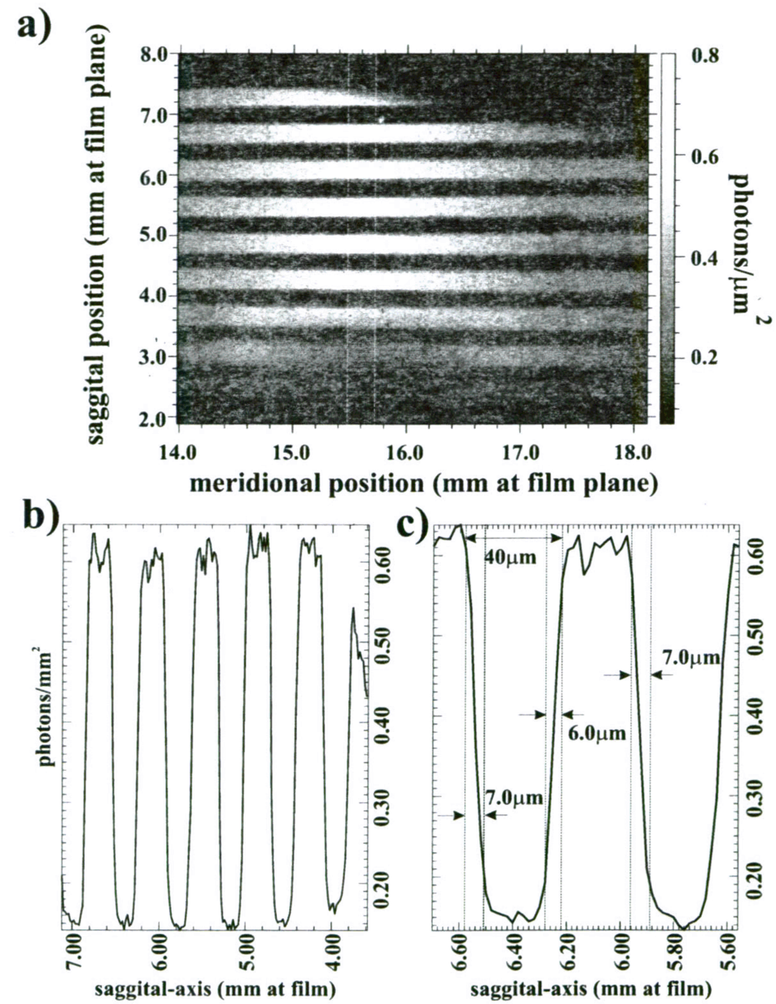






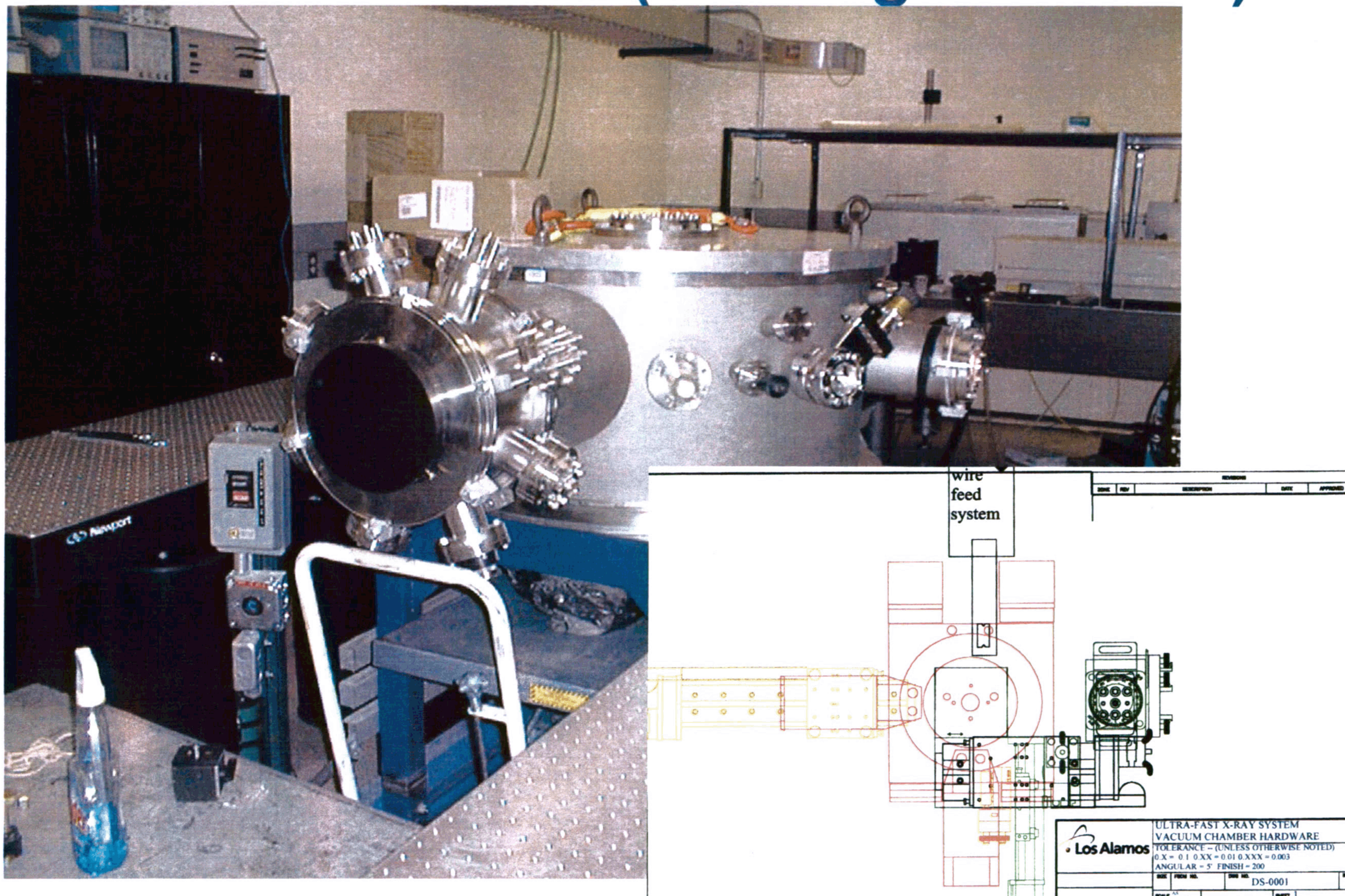
Previous Work at LANL Demonstrated 6-7μm Resolution Imaging with Spherical Crystals at 4.75 keV



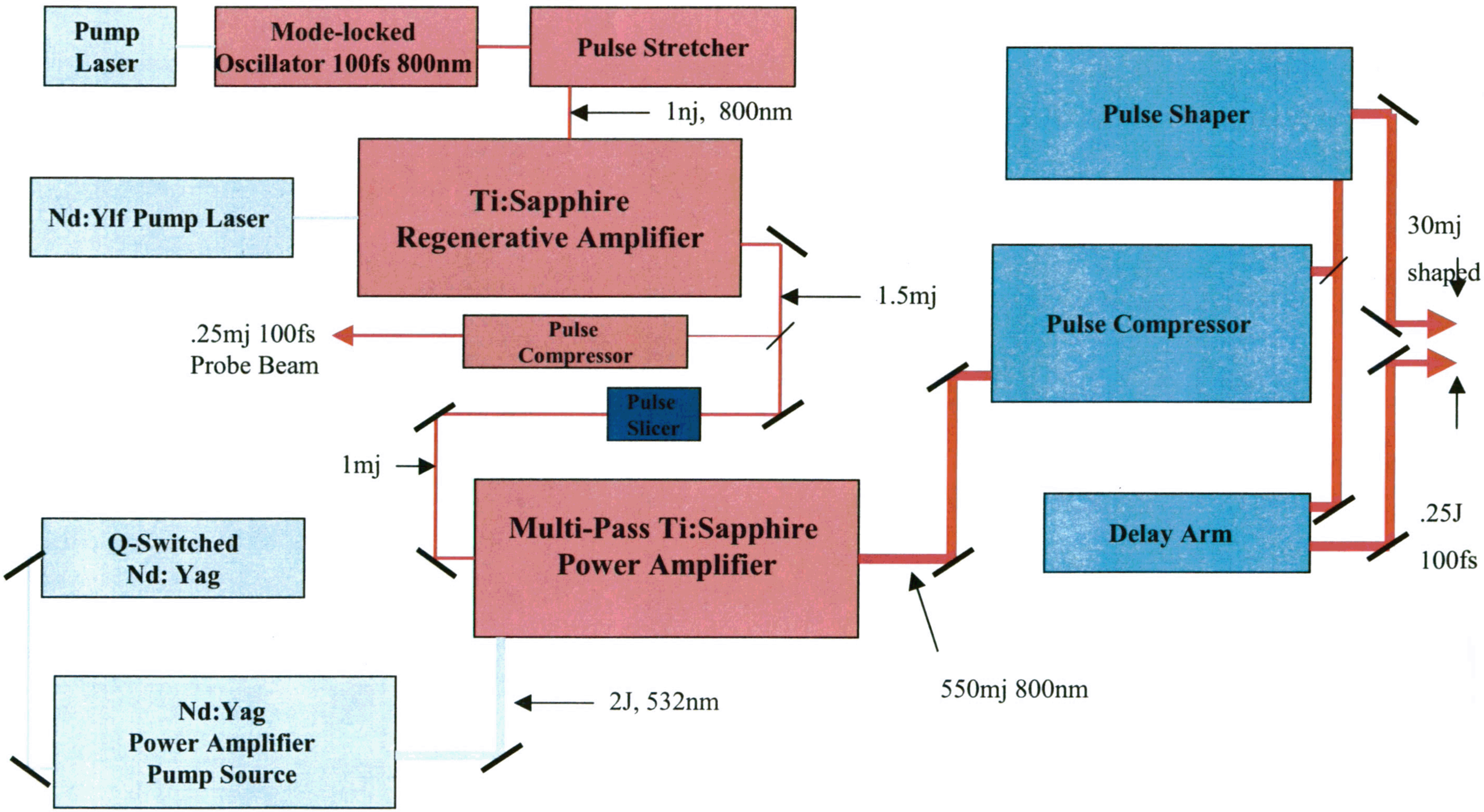


J. Workman, S. Evans and G.A. Kyrala, Rev Sci. Instr. 72, 674 (2001).

Diffraction Chamber (old Bright Source)

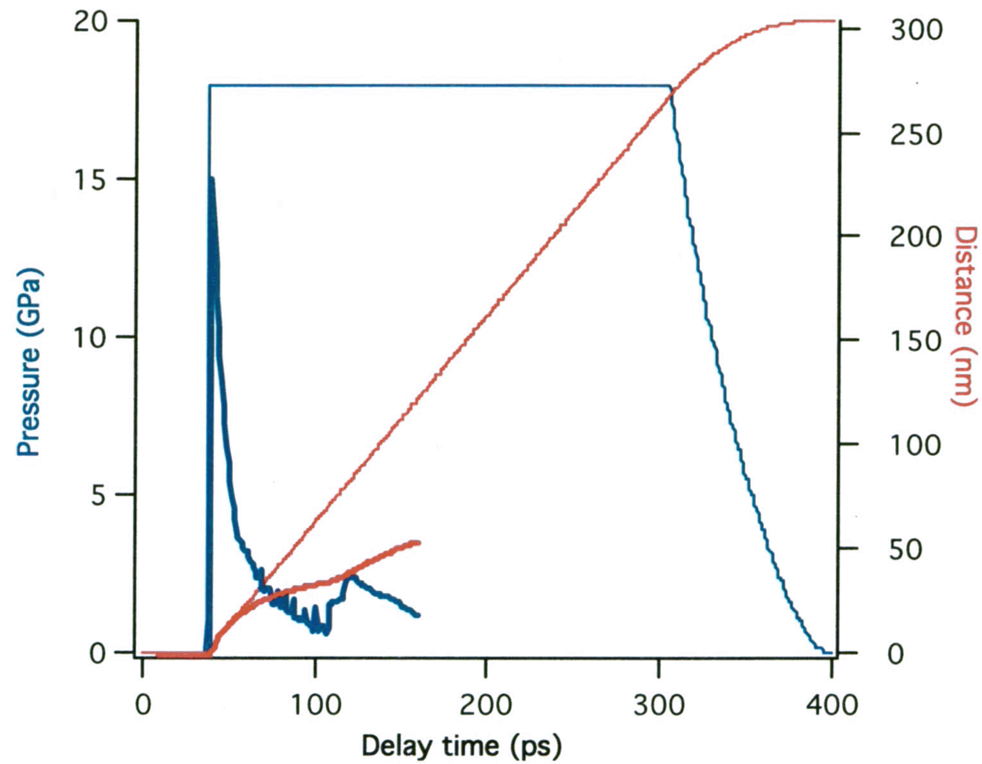


All Solid State Terawatt Laser System



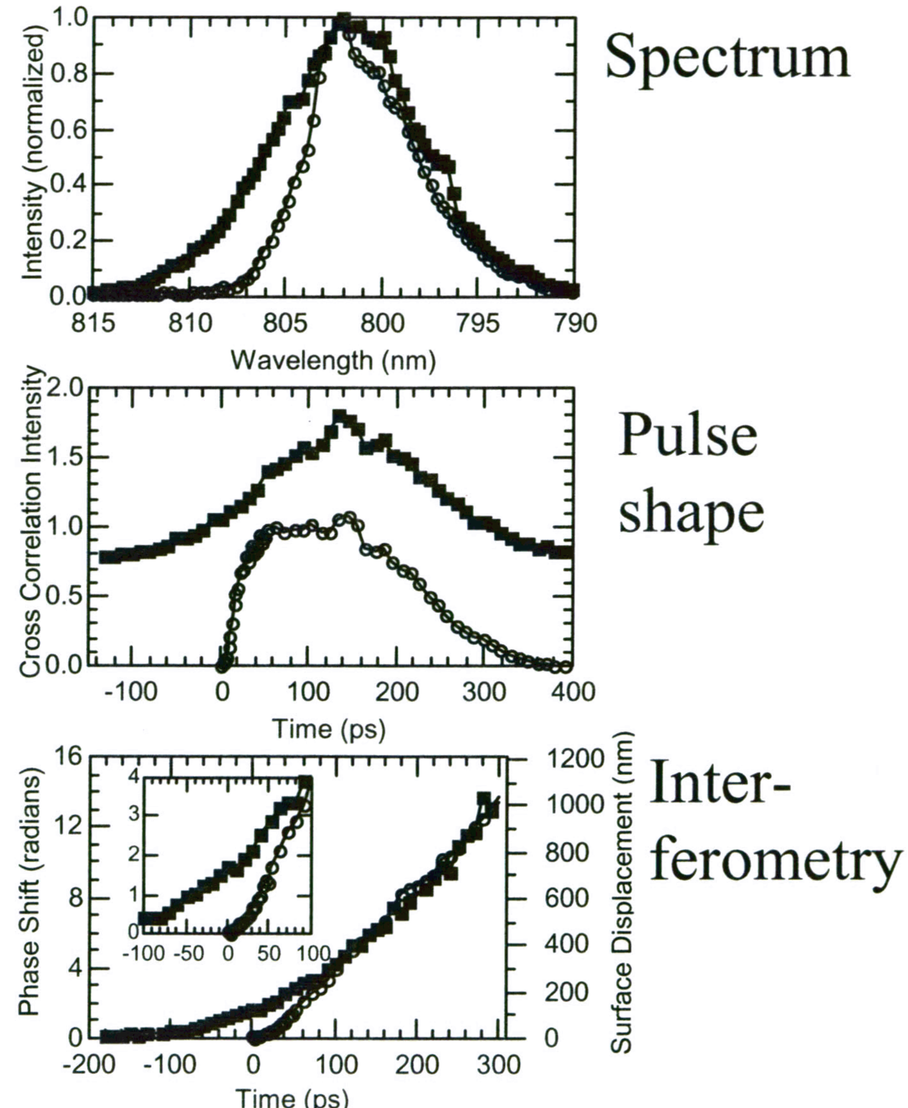
The Shape of the Drive Pulse is Important

- 130 fs drive laser pulse (dotted)
  - Shocks are not supported
  - Shock strength decreases with run distance
  - Pressure wave is triangular (few ps rise, 30-40 ps fall)
- What shock shape do we want?
  - Sharp rise (few ps - limited by material response)
  - Constant pressure for > 200 ps
  - Usually accomplished via support (simulation is 1 μm thick flyer - solid curves)



We have Generated a Sharply Rising Pulse Shape Suitable for Driving Shocks

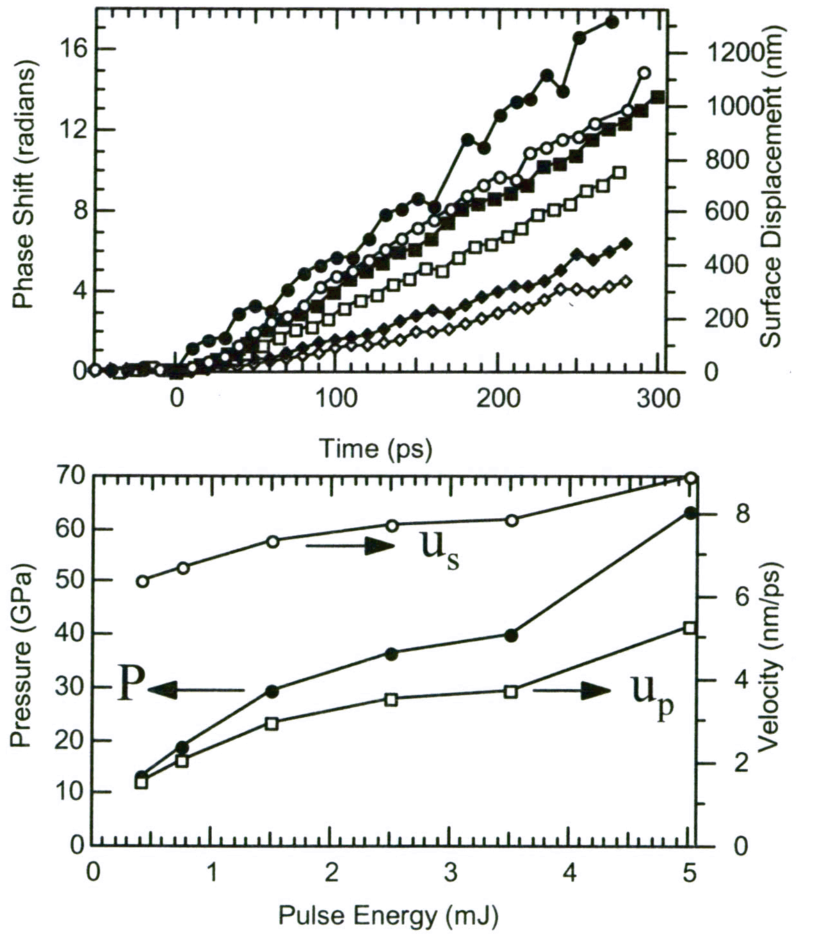
- Laser amplifier utilizes a pulse stretcher and compressor (CPA)
- Red spectral end of pulse exits stretcher first
- Therefore
  - Block red spectral end of stretched pulse
  - Use uncompressed pulse to drive shock
- Compress rest of pulse for spectroscopy/diagnostics



Los Alamos

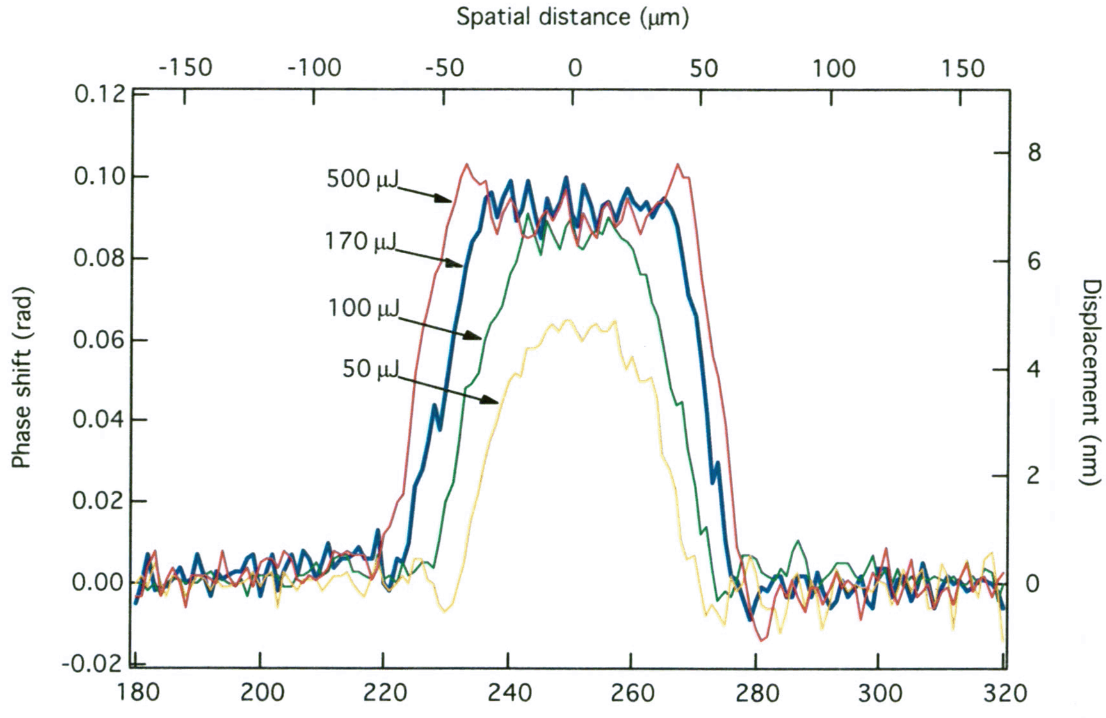
High Shock Pressures can be Sustained

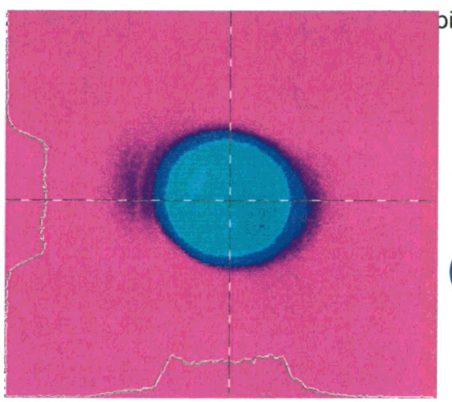
- Shaped long drive pulse allows us to adjust pressure
  - 120 fs drive pulse was optically limited in substrate
- 0.6 Mbar achievable
- Pressure can be sustained for > 250 ps
- Diffraction interpretation simplified by nearly isobaric conditions behind shock
- S.D. McGrane, D. S. Moore, D. J. Funk and R. L. Rabie, Appl. Phys. Lett., 80(21), 3919 (2002).



Long Pulse Drive is not Spatially Planar (yet)

- 120 fs shock drive pulse through 150 μm thick glass substrate gives extremely planar shocks
- Shaped long drive pulse gives only Gaussian spatial profile to date
- Preflatten in sapphire
  - Occurs at fluences ten times below the damage threshold
- Then stretch and spectrally modify

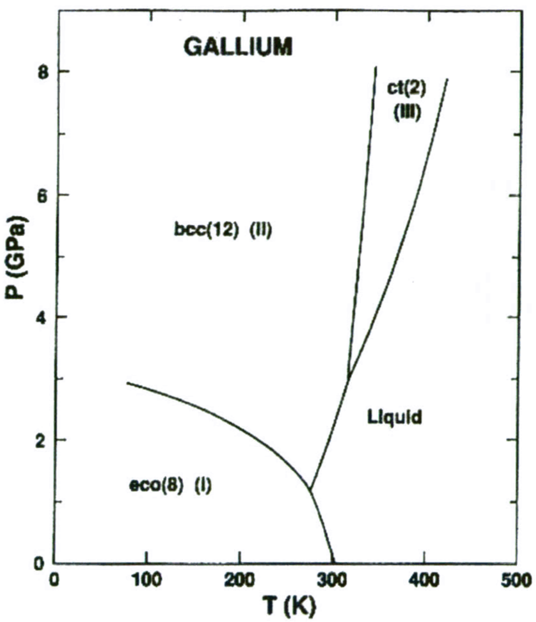


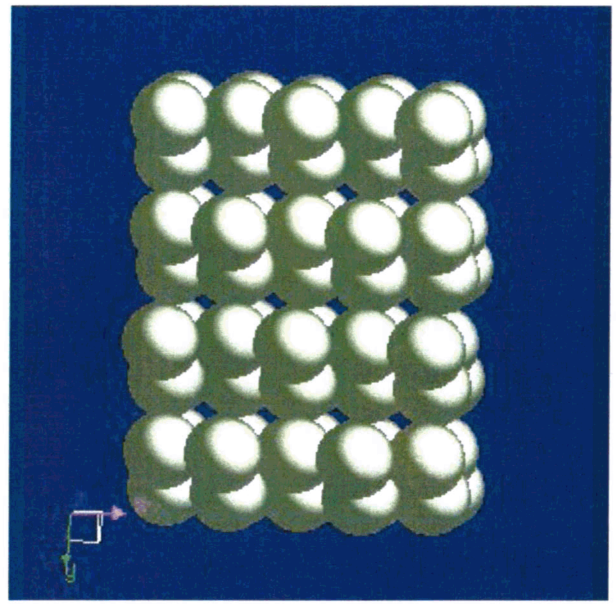


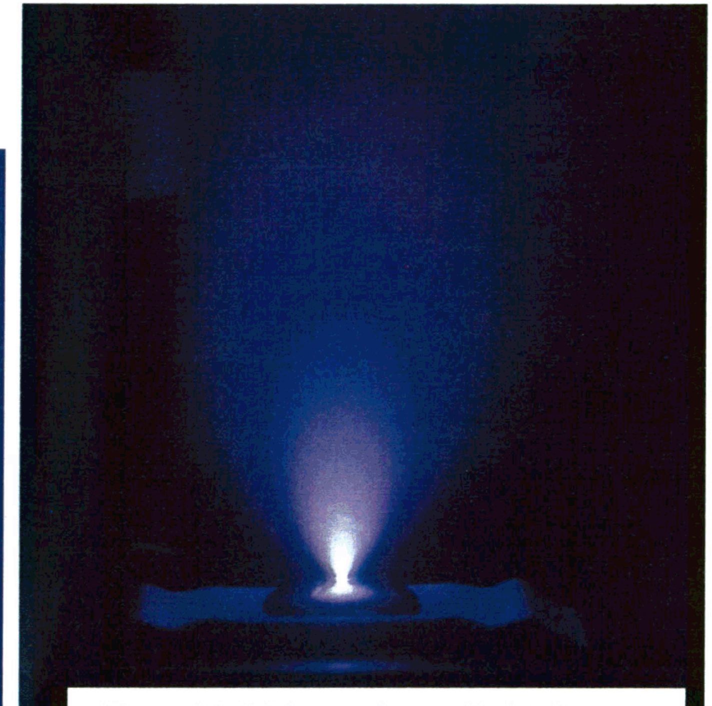
120 fs
1 mm path
0.43 J/cm^2

Los Alamos

First Material to Study under Shock Loading: Gallium







•Use of 1.064 mm laser light for ablation of gallium

–MacDonald et al. (J. Opt. Soc. Am. B. 18(3) 331 [2001])

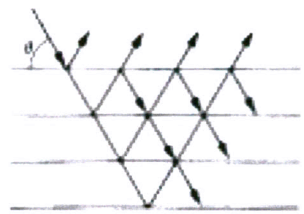
–Prepared thin films of alpha gallium on quartz substrates

–Cycled multiple times through melt with no change in behavior

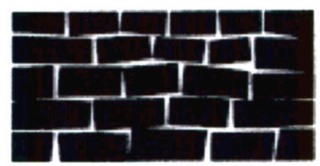
- Crystal Properties
  - Base-centered orthorhombic (a = 451.97 pm, b= 766.33 pm, c= 452.6 pm)
- Melts at moderate shock pressure (5-10 kbar)

Dynamical vs. Kinematic Diffraction Theory (from B. E. Warren, X-ray Diffraction)

Perfect Crystal

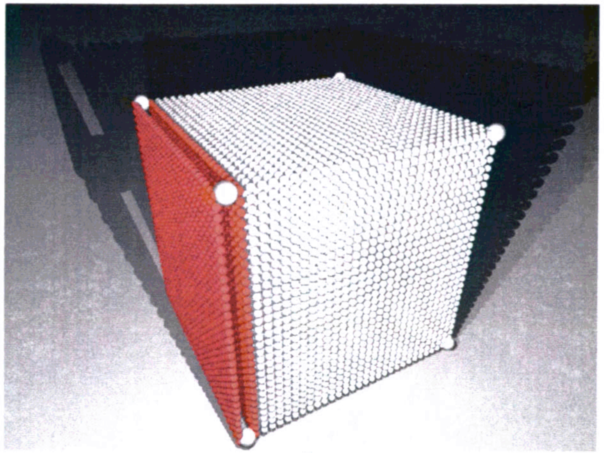


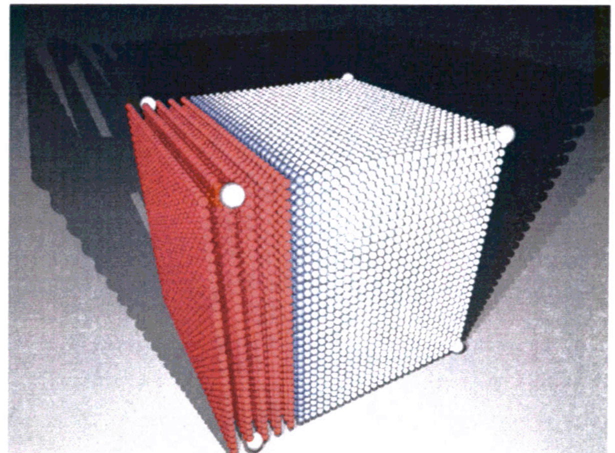
Mosaic

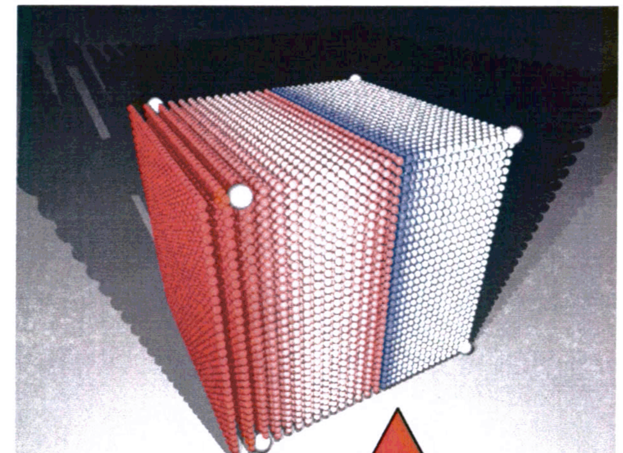


Shocked Crystal

Coherent Acoustic Phonons







Fast heating at constant Volume

Stress

Surface expansion

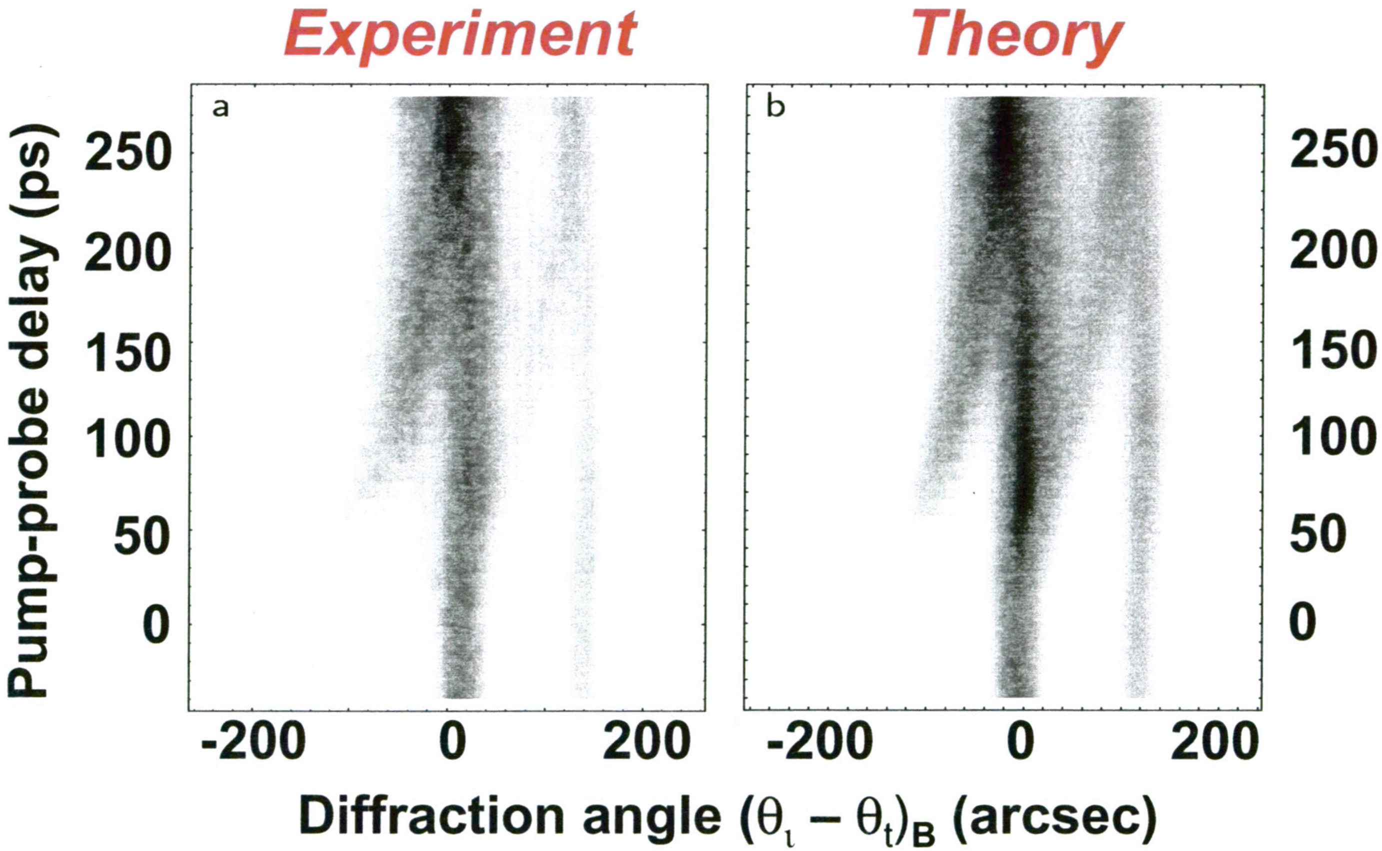
Strain

Newton's 3rd Law

Acoustic Pulse

C. Thomsen et al. Phys Rev. B 34, 4129 (1986)

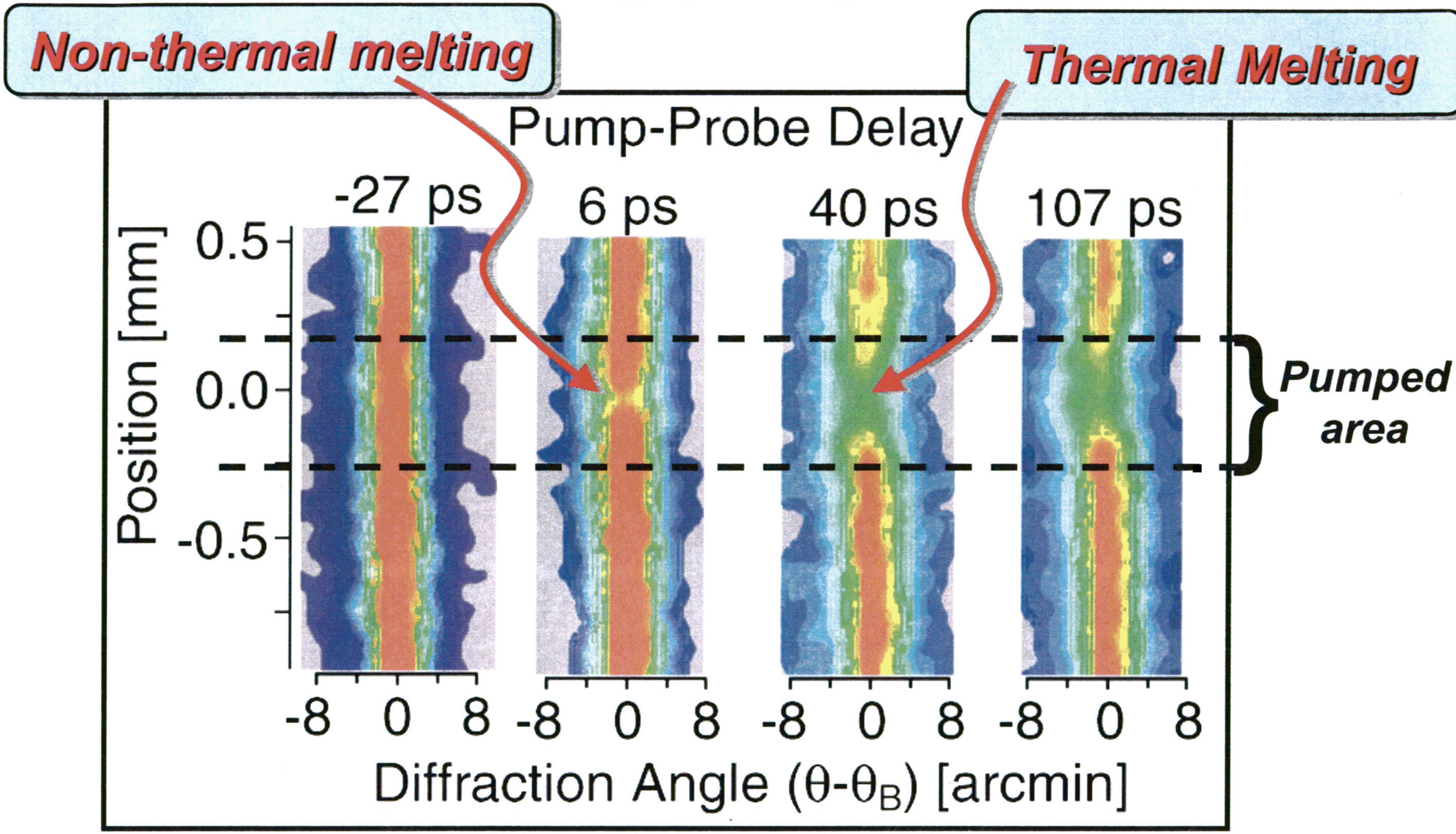
Coherent Acoustic Phonons



Milliångström lattice dynamics with picosecond resolution

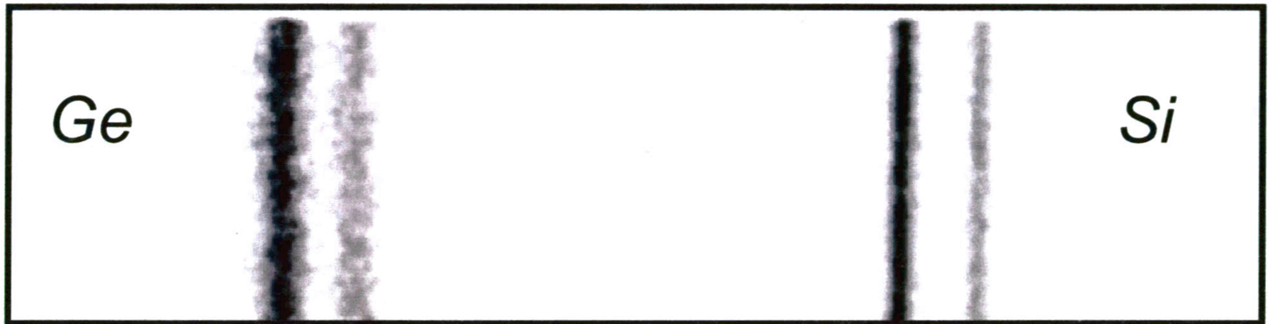
Ch. Rose-Petruck et al. "Picosecond milliångström lattice dynamics measured by ultrafast X-ray diffraction" Nature 398, 310 (1999)

Ultrafast Melting (X-ray Probe) in Ge



C.W. Siders et al.,
Science <u>286</u>, 1340 (1999)

Probing Buried Interfaces



Ge (400 nm): expansive strain d/c_L $2\ d/c_L$

Si: compressive strain d/c_L $2\ d/c_L$